

# Computation of Shock Waves in Inert Binary Diatomic Gas Mixtures in Non-equilibrium Using the Generalized Boltzmann Equation

Geng Qian<sup>1</sup>, Ramesh K. Agarwal<sup>\*2</sup>, Christopher D. Wilson<sup>3</sup>

Beijing Institute of Technology, Beijing 100081, China; Washington University in St. Louis, Missouri 63130, USA;  
Boeing Company, St. Louis, MO 63166, USA

<sup>1</sup>gloria716@gmail.com; <sup>\*2</sup>rka @wustl.edu; <sup>3</sup>christopher.d.wilson.pe@gmail.com

## Abstract

For numerical solution of the Generalized Boltzmann Equation (GBE) for simulating rarefied hypersonic flows in a gas mixture of multiple species, the GBE is formulated in the impulse space. The gas mixtures may consist of both monatomic and diatomic gases with arbitrary constituents, concentrations, and mass ratios. The conservative discrete ordinates method of Tcheremissine is applied to validate the solutions against the existing simulations for shock waves in an inert binary mixture of monoatomic gases. The method is then exercised for various concentration ratios, mass ratios, and density ratios to evaluate its ability to simulate a wide range of binary gas mixtures of monoatomic and diatomic gases. In particular, the method is applied to simulate two of the three primary constituents of air ( $N_2$ ,  $O_2$ , Ar) in a binary mixture at 1:1 density ratio and air concentration ratio with gases in translational, rotational and vibrational non-equilibrium. The solutions presented in the paper can serve as validation test cases for other methods as well as an important building block in developing complex 3D simulations for shock waves in a mixture of multiple gases.

## Keywords

Generalized Boltzmann Equation; Non-equilibrium Hypersonic Flows; Shock Waves in Inert Gas Mixtures; Rotational and Vibrational Non-equilibrium Flows

## Nomenclature

$\rho_A$  = Density of gas A

$\rho_B$  = Density of gas B

$m_A$  = Mass of gas A

$m_B$  = Mass of gas B

$d_A$  = Molecular diameter of gas A

$d_B$  = Molecular diameter of gas B

$P_A$  = Pressure of gas A

$P_B$  = Pressure of gas B

$U_A$  = Velocity of gas A

$U_B$  = Velocity of gas B

$T_A$  = Translational temperature of gas A

$T_B$  = Translational temperature of gas B

$T_{xA}$  = Longitudinal component of translational temperature of gas A

$T_{xB}$  = Longitudinal component of translational temperature of gas B

$T_{yA}$  = Transverse component of translational temperature of gas A

$T_{yB}$  = Transverse component of translational temperature of gas B

$T_{rot, A}$  = Rotational temperature of gas A

$T_{rot, B}$  = Rotational temperature of gas B

$T_{vib, A}$  = Vibrational temperature of gas A

$T_{vib, B}$  = Translational temperature of gas B

M = Mach number

Note: A and B can be  $N_2$ ,  $O_2$  or Ar

## Introduction

A goal of continued development of direct methods for solving the generalized Boltzmann equation (GBE) is to extend the existing GBE solver to calculate the flowfields of inert gas mixtures of monatomic and diatomic gases in translational, rotational and vibrational non-equilibrium. The GBE is a modification of the Wang-Chang Uhlenbeck equation to include the degenerate energy levels for the internal degrees of freedom. The solution of GBE for a single specie diatomic gas was first obtained by Tcheremissine. In recent years, the authors have

collaborated with Tcheremissine to develop 3D solvers for both the Classical Boltzmann Equation (CBE) and the Generalized Boltzmann Equation (GBE) to compute the hypersonic non-equilibrium flows past blunt bodies. This paper describes further development and application of these solvers for computing hypersonic shock waves flows in a binary mixture of inert gases. In general, many gas mixtures include a large number of species, which may also be reacting. Both the CBE and GBE solvers employ conservative discrete ordinates method developed by Tcheremissine for the solution of collision integral.

For computing the hypersonic shock waves in an inert binary mixture of monatomic and diatomic gases, the Boltzmann equation is reformulated in the impulse space. The developed code is first validated by computing the shock wave solutions in an inert mixture of two monatomic gases for which computations of Kosuge et al. are available. The code is then employed to compute shock waves in a binary inert gas mixture of a monoatomic gas for a range of concentration ratios, diameter ratios, and mass ratios. The mixture is considered to be in translational non-equilibrium only. Finally, the code is employed to compute shocks in a binary gas mixture of monoatomic and diatomic gases; the gases are considered to be in translational, rotational and vibrational non-equilibrium. The gases considered are the primary constituents of air ( $N_2$ ,  $O_2$ , Ar). It is important to note that the first attempt to solve the Classical Boltzmann Equation (CBE) for a mixture of monoatomic gases was made by Raines.

### Shock Wave Simulations in Binary Inert Gas Mixtures

So far in the existing literature, direct methods for the solution of the classical Boltzmann equation have only been employed for the computation of shock structures in an inert mixture of two monatomic gases with varying concentrations and for a mixture of two monoatomic/diatomic gases in translational non-equilibrium only.

Wilson et al. computed the shock structure in an inert binary mixture of two diatomic gases in translational non-equilibrium at Mach 5; however, they recognized that the inclusion of both the rotational and vibrational energy levels in the calculation of shock structure would be very computationally intensive. Therefore, Tcheremissine et al. developed and validated a two-level rotational energy (2LRT) model for the solution

of the GBE for RT relaxations. By introducing the 2LRT model, Tcheremissine and Agarwal were able to reduce the total number of rotational and vibrational energy levels from 420 to 12 for a Mach 10 shock in a gas in both rotational and vibrational non-equilibrium. The natural extension of the work of Wilson et al. is to consider a binary mixture of a monoatomic gas such as Ar and a diatomic gas such as  $N_2$  and a binary mixture of two diatomic gases such as  $N_2$  and  $O_2$  in translational, rotational and vibrational non-equilibrium. The focus of this paper is on this extension and computations.

### *Comparison of Present Solutions with Existing Computations for a Binary Mixture of Monoatomic Gases*

Kosuge et al. have presented a detailed evaluation of the properties of one-dimensional shock waves in inert binary gas mixtures of monoatomic gases. They presented the results of several simulations and included tabulated data for two of the simulations. Two pairs of Mach numbers and mass ratios were considered – Mach 2 with a mass ratio of 0.25 and Mach 3 with a mass ratio of 0.5. Examples of the results are shown in Fig. 1 at Mach 2 for constituent B (concentration equal to 0.1) and a mass ratio equal to 0.25. Figure 2 presents the results at Mach 3 for constituent B (concentration equal to 0.1) and a mass ratio equal to 0.5. Figure 1(a) and 2(a) show the comparison of the present results for the mixture with those of Kosuge et al. at  $M = 2$  and  $M = 3$  respectively. Based upon these comparisons, it can be concluded that the current approach produces solutions in good agreement with the results obtained by Kosuge et al. Figures 1(b) and 2(b) show the behaviour of properties for each constituent and the mixture through the shock wave at  $M = 2$  and  $M = 3$  respectively.

### *Parametric Study of Shock Structure in Binary Gas Mixtures of Monoatomic Gases*

As demonstrated in the preceding section, the present numerical approach shows good agreement with the results of Kosuge et al. obtained by using the numerical method of Sone for the collision integral. In this section, we further demonstrate the solution capability of the present method by performing simulations for a range of mass ratios, diameter ratios, and density ratios. Five values for each ratio are used (0.1, 0.5, 1.0, 5.0, and 10). A total of thirteen simulations are performed at Mach 2. Some of these results are shown in Figs. 3 - 5. Figure 3 shows the

baseline solution for Mach 2 where each ratio is equal to unity. The solutions that were generated by varying only the concentrations of each constituent in the binary mixture resulted in similar solutions since the mass and diameter ratios of the constituents A and B were equal to unity. As expected, these solutions produced results similar to those shown in Fig. 3.

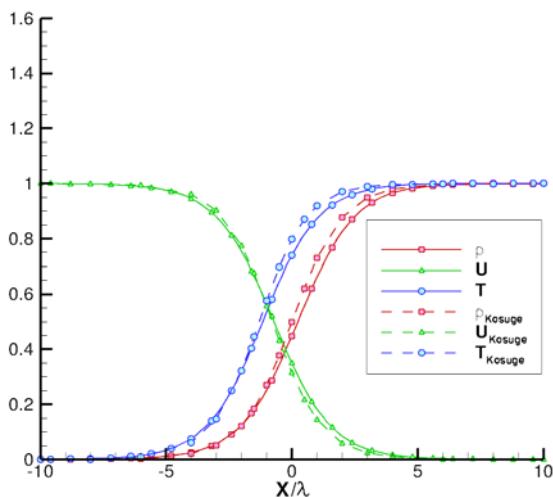


FIG. 1(a) SHOCK WAVE PROPERTIES AND THEIR COMPARISON WITH THE COMPUTATIONS OF KOSUGE ET AL.; GAS B CONCENTRATION = 0.1, MASS RATIO = 0.25, M = 2

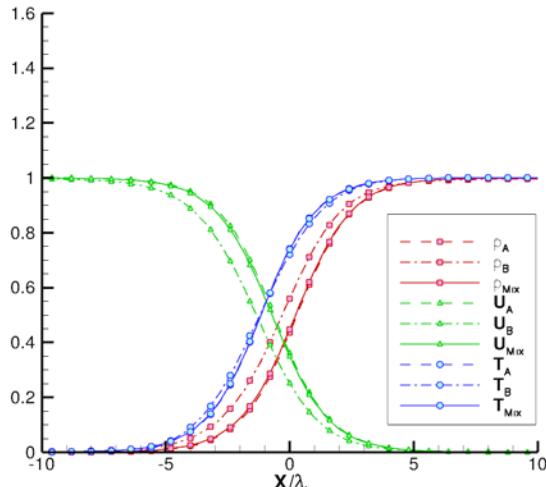


FIG. 1(b) SHOCK WAVE PROPERTIES OF EACH CONSTITUENT A AND B AND THE MIXTURE; GAS B CONCENTRATION = 0.1, MASS RATIO = 0.25, M = 2

An example of the solutions for the non-unity mass ratios is presented in Fig. 4. These solutions demonstrate that as the mass of a constituent becomes lighter, with respect to the other constituent in the mixture, the lighter constituent begins to experience changes in its properties further upstream than the heavier constituent. Another important note from the mass ratio parametric study is that extremely small mass ratios ( $m_B/m_A = 0.1$ ) or extremely large mass ratios ( $m_B/m_A = 10$ ) require smaller time steps in

order to obtain convergent solutions.

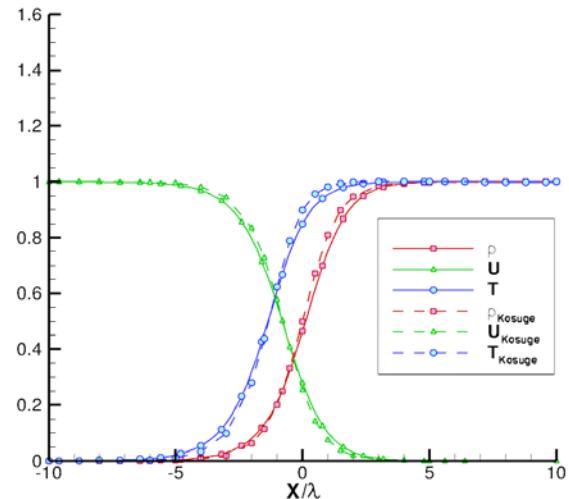


FIG. 2(a) SHOCK WAVE PROPERTIES AND THEIR COMPARISON WITH THE COMPUTATIONS OF KOSUGE ET AL.; GAS B CONCENTRATION = 0.1, MASS RATIO = 0.5, M = 3

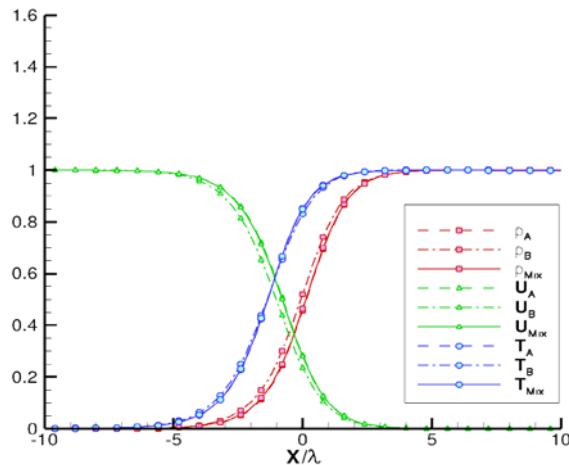


FIG. 2(b) SHOCK WAVE PROPERTIES OF EACH CONSTITUENT A AND B AND THE MIXTURE; GAS B CONCENTRATION = 0.1, MASS RATIO = 0.5, M = 3

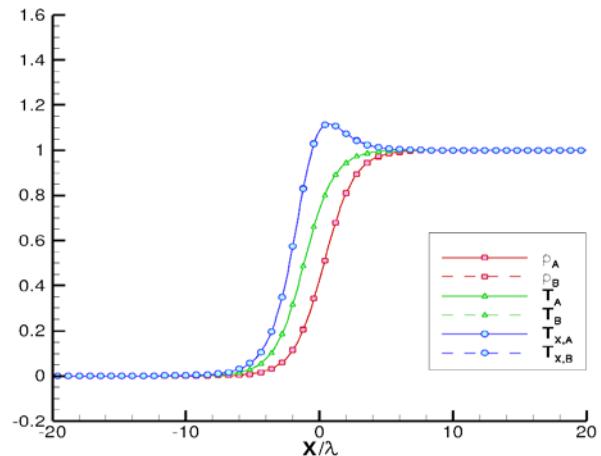


FIG. 3(a) BASELINE SHOCK STRUCTURE PROPERTIES OF TWO CONSTITUENTS A AND B IN A BINARY GAS MIXTURE AT M = 2;  $m_B/m_A = 1$ ,  $d_B/d_A = 1$

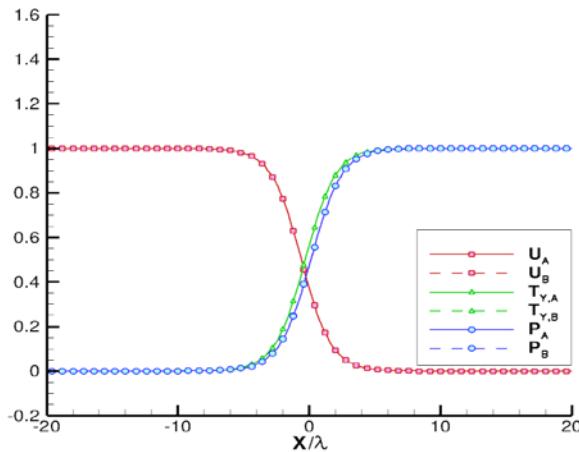


FIG. 3(b) BASELINE SHOCK STRUCTURE PROPERTIES IN A BINARY GAS MIXTURE OF TWO CONSTITUENTS A AND B AT  $M = 2$ ;  $m_B/m_A = 1$ ,  $dB/dA = 1$

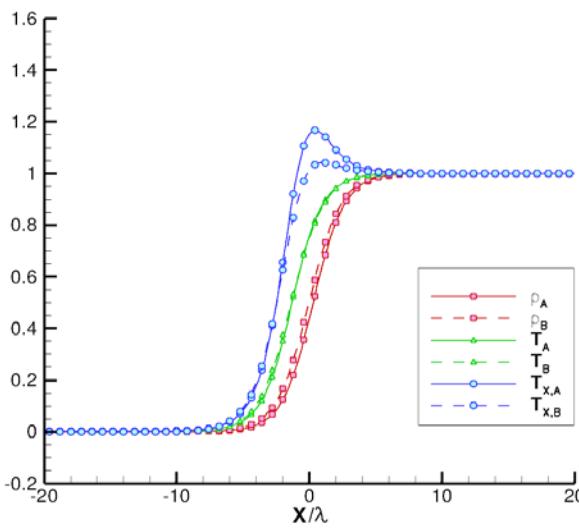


FIG. 4(a) SHOCK STRUCTURE PROPERTIES IN A BINARY GAS MIXTURE OF TWO CONSTITUENTS A AND B WITH  $m_B/m_A = 0.5$  AND  $dB/dA = 1$  AT  $M = 2$

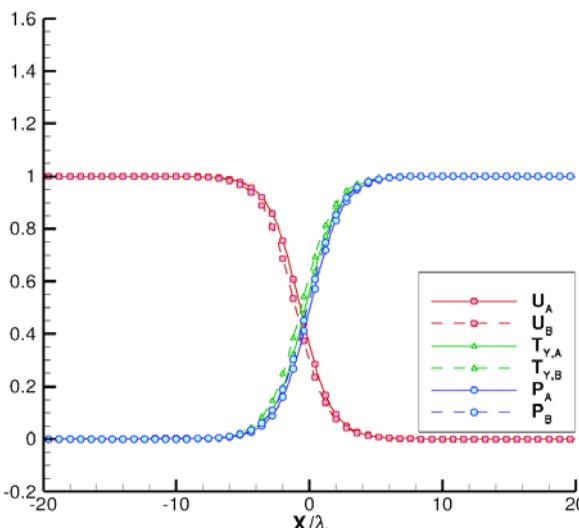


FIG. 4(b) SHOCK STRUCTURE PROPERTIES IN A BINARY GAS MIXTURE OF TWO CONSTITUENTS A AND B WITH  $m_B/m_A = 0.5$  AND  $dB/dA = 1$  AT  $M = 2$

An example of the solutions for the non-unity diameter ratios is presented in Fig. 5. These solutions demonstrate that, when the diameter ratio of two constituents becomes significantly different from unity, the thickness of the shock increases. Furthermore, the smaller diameter constituent, with respect to the other constituent in the mixture, begins to experience changes in its properties earlier than the larger diameter constituent.

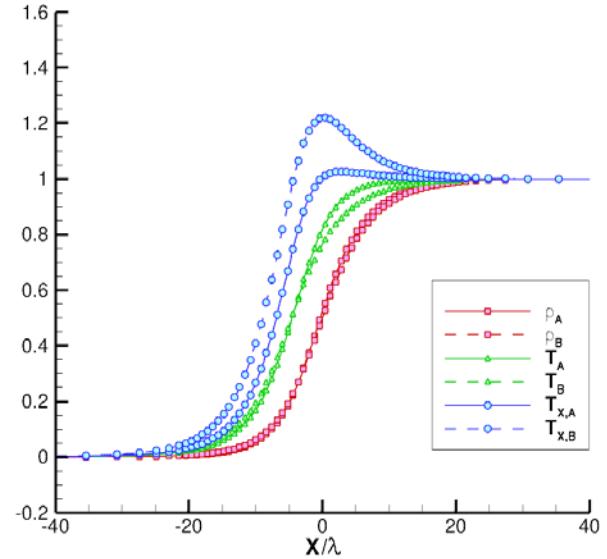


FIG. 5(a) SHOCK STRUCTURE PROPERTIES IN A BINARY GAS MIXTURE OF CONSTITUENTS A AND B WITH  $m_B/m_A = 1$  AND  $dB/dA = 0.1$  AT  $M = 2$

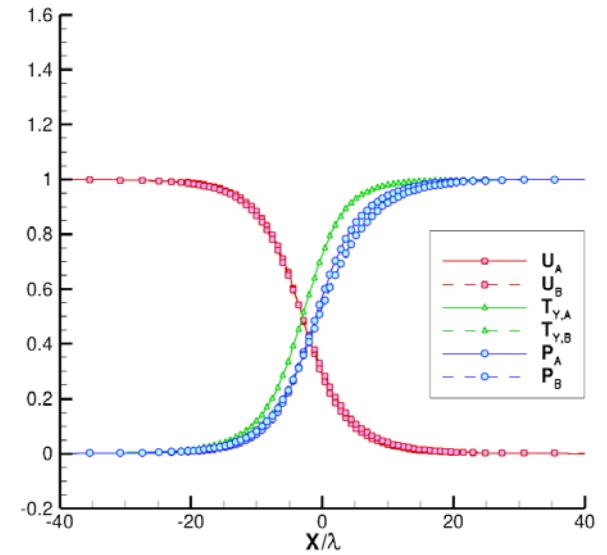


FIG. 5(b) SHOCK WAVE PROPERTIES IN A BINARY GAS MIXTURE OF CONSTITUENTS A AND B WITH  $m_B/m_A = 1$  AND  $dB/dA = 0.1$  AT  $M = 2$

The parametric study performed in this section demonstrates that the code is able to handle molecular constituent properties that are far from unity. For the application to immersed bodies, the most relevant gas

mixture is air. As a gas mixture, air is relatively well conditioned for the present code since it has mass and diameter ratios of different constituents close to unity. The next section presents the behavior of a one-dimensional shock wave for a binary gas mixture comprised of two of the three primary constituent of air ( $N_2$ ,  $O_2$ , Ar).

### **Shock Wave Solutions for Binary Gas Mixture of Air Constituents in Translational Non-equilibrium**

Historically, there are hardly any solutions for shock waves in a mixture of gases representative of the constituents of air. Furthermore, simulations of gas mixtures have been limited to two constituents of similar atomic structure (i.e. two diatomic gases or two monatomic gases). This section presents solutions for binary mixtures of two of the three primary constituents of air at 1:1 concentration and concentrations representative of those in air. Table 1 presents a summary of the key parameters used in the simulations. The Van der Waals radius can be used to approximate the diameter of the molecule in the collision integral. The rotational and vibrational degrees of freedom for Argon can be neglected since it is monatomic. A solution for each mixture was generated at Mach 2 and Mach 5. All Figures presented in this section are for the Mach 5 shock wave for the concentration ratios as found in the air. All constituent gases are assumed to be non-reacting.

TABLE 1 GAS MIXTURE PROPERTIES FOR AIR

Constituent	Mole Fraction	Atomic Weight	Van der Waals Radius
$N_2$	0.78084	28.0134(4)	225
$O_2$	0.20946	31.9988(6)	206
Ar	0.00934	39.948(1)	188

#### **1) $N_2$ and $O_2$ Mixture**

The first binary mixture of air constituents considered is that of  $N_2$  and  $O_2$  in translational non-equilibrium only. The mass ratio equals 1.1423 and the diameter ratio equals 0.9156. The solutions for the 1:1 concentration reaffirm the conclusion drawn from the parametric study in the previous section that the lighter constituent ( $N_2$ ) begins experiencing changes in properties earlier in the shock wave structure. Additionally, the change in concentration ratio does not have a significant

impact on the shock structure. Figure 6 presents an example of the results for  $N_2$  and  $O_2$ .

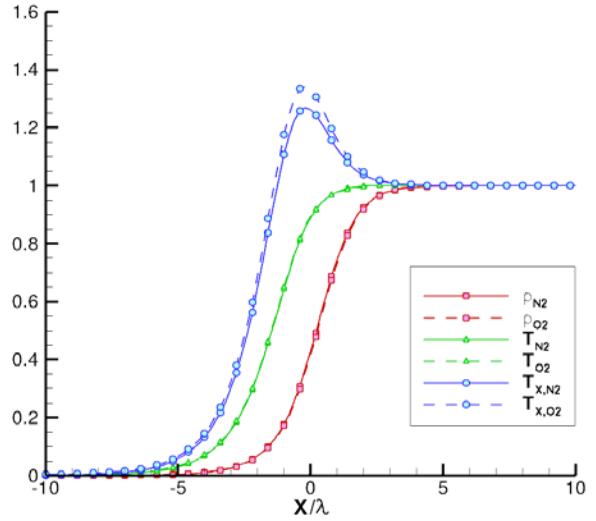


FIG. 6(a) SHOCK WAVE PROPERTIES IN A MIXTURE OF NITROGEN AND OXYGEN (AS IN AIR) AT  $M = 5$

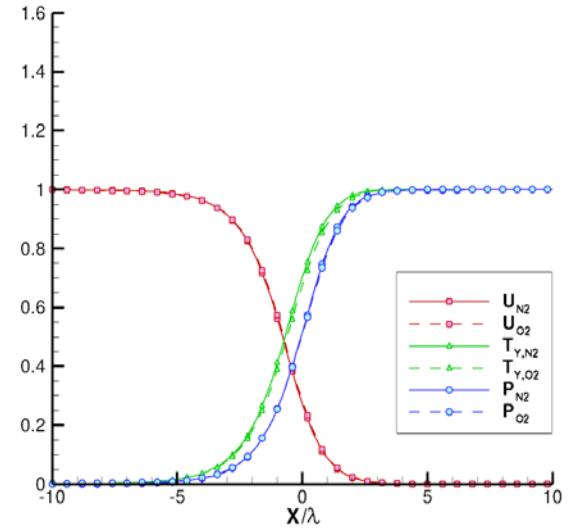


FIG. 6(b) SHOCK WAVE PROPERTIES IN A MIXTURE OF NITROGEN AND OXYGEN (AS IN AIR) AT  $M = 5$

#### **2) $N_2$ and Ar Mixture**

The second binary mixture of air constituents considered is that of  $N_2$  and Ar (a diatomic and a monoatomic gas respectively). The mass ratio equals 1.4260 and the diameter ratio equals 0.8356. The gases are assumed to be non-reacting and again in translational non-equilibrium. It is interesting to note that the shock thickness has increased compared to that in  $N_2/O_2$  mixture simulation. This increase can be attributed to the change in the diameter ratio, as also noted in the previous section on parametric study. Additionally, the tendency for the lighter constituent to begin experiencing changes earlier in the shock wave

holds. Figure 7 presents an example of the results for N<sub>2</sub> and Ar.

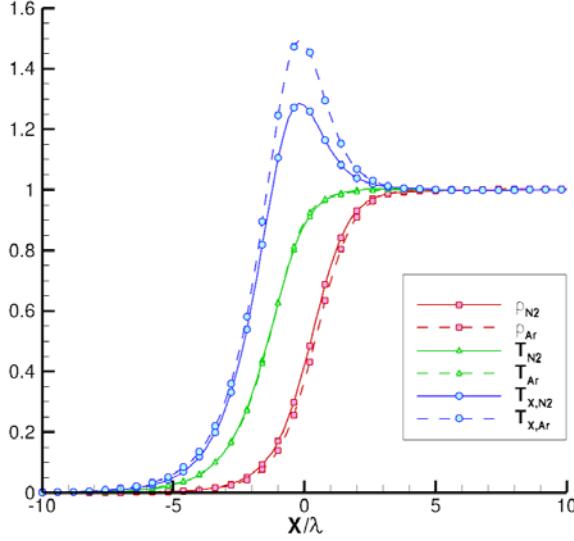


FIG. 7(a) SHOCK WAVE PROPERTIES IN A MIXTURE OF NITROGEN AND ARGON (AS IN AIR) AT M = 5

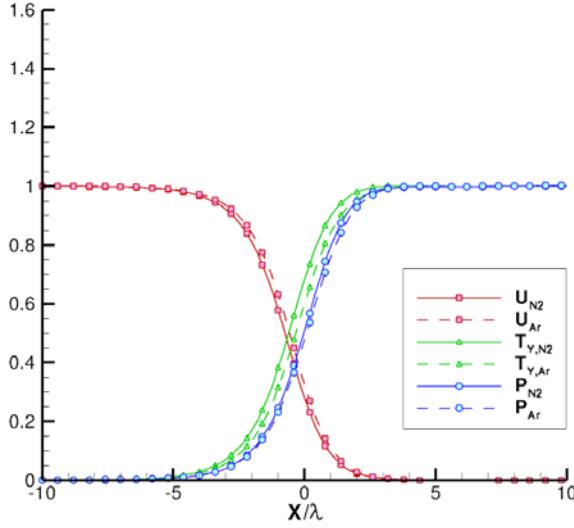


FIG. 7(b) SHOCK WAVE PROPERTIES IN A MIXTURE OF NITROGEN AND ARGON (AS IN AIR) AT M = 5

### 3) O<sub>2</sub> and Ar Mixture

The third binary mixture of air constituents considered is that of O<sub>2</sub> and Ar. The mass ratio equals 1.2484 and the diameter ratio equals 0.9126. The results for these simulations are similar to those obtained from the N<sub>2</sub>/Ar mixture simulation. The shock wave thickness is greater than that obtained from the N<sub>2</sub>/O<sub>2</sub> mixture simulation. One would not expect the shock wave thickness to be significantly different between the N<sub>2</sub>/Ar simulation and the O<sub>2</sub>/Ar simulation since the diameter ratios are similar. Additionally, O<sub>2</sub> is the lighter gas compared to Argon. Therefore, O<sub>2</sub> has a tendency to experience changes in constituent

properties earlier in the shock, as demonstrated previously. Figure 8 presents an example of the results for O<sub>2</sub> and Ar.

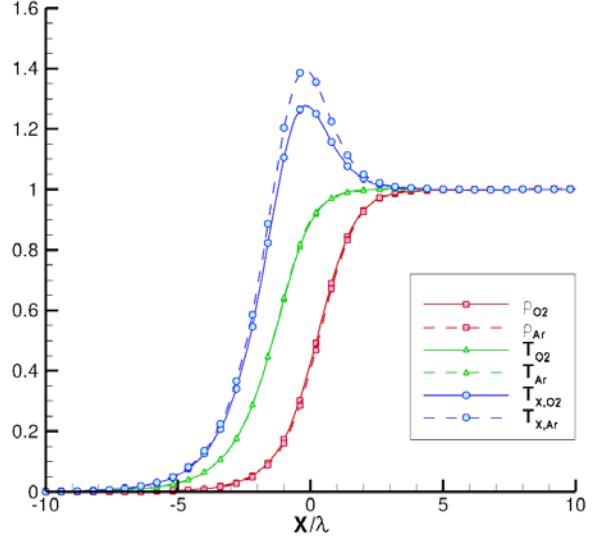


FIG. 8(a) SHOCK WAVE PROPERTIES IN A MIXTURE OF OXYGEN AND ARGON (AS IN AIR) AT M = 5

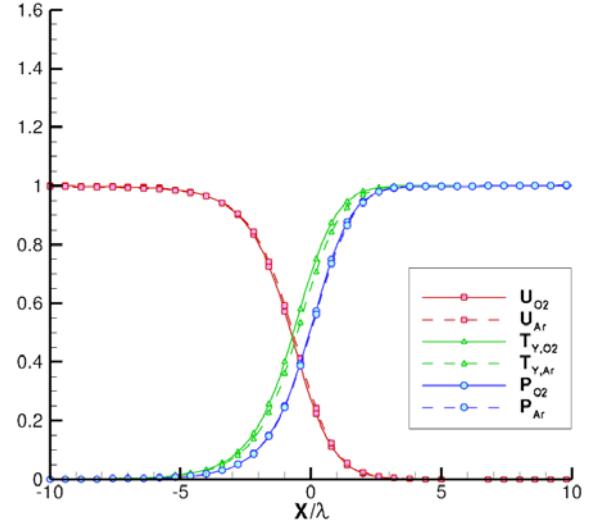


FIG. 8(b) SHOCK WAVE PROPERTIES IN A MIXTURE OF OXYGEN AND ARGON (AS IN AIR) AT M = 5

### Shock Wave Solutions for Binary Gas Mixture of N<sub>2</sub> and Ar, and N<sub>2</sub> and O<sub>2</sub> in Translational and Rotational Non-equilibrium

#### 1) N<sub>2</sub> and Ar Mixture

This case is the same as that shown in Fig. 7 except that N<sub>2</sub> is in both the translational and rotational non-equilibrium while Ar is in translational non-equilibrium only. The mass ratio equals 1.4260 and the diameter ratio equals 0.8356. The gases are again assumed to be non-reacting. Figure 9 shows various flow properties for the two gases at Mach 2 with concentration as in air. Again as shown before

in Fig. 7, N<sub>2</sub> being lighter than Ar, it experiences changes in the shock properties earlier than Ar. However it is important to note that the peak of the longitudinal component of the translational temperature for Ar is much higher than that for N<sub>2</sub> in this case compared to that in Fig. 7. This effect is due to transfer of rotational energy of N<sub>2</sub> into the translational energy of Ar. Figure 10 shows various flow properties for the two gases at Mach 5 with 1:1 concentration ratio. Again the behavior of change in shock properties is the same as that in Fig. 9 except that the peaks of normalized longitudinal temperatures of the two gases are smaller than those in Fig. 9 as expected.

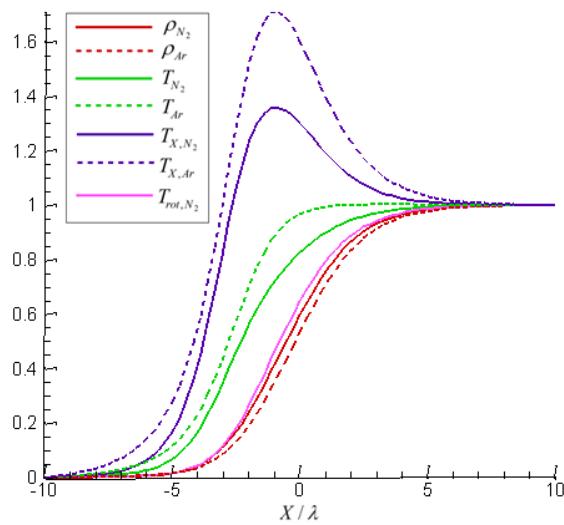


FIG. 9(a) SHOCK WAVE PROPERTIES IN A MIXTURE OF NITROGEN AND ARGON IN TRANSLATIONAL AND ROTATIONAL NON-EQUILIBRIUM WITH AIR CONCENTRATION AT M = 2

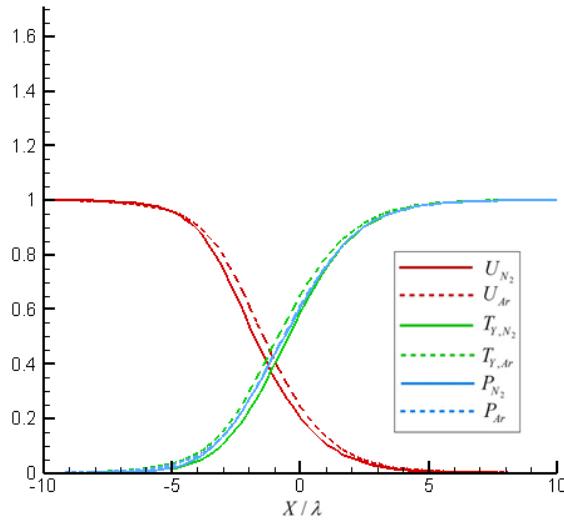


FIG. 9(b) SHOCK WAVE PROPERTIES IN A MIXTURE OF NITROGEN AND ARGON IN TRANSLATIONAL AND ROTATIONAL NON-EQUILIBRIUM WITH AIR CONCENTRATION AT M = 2

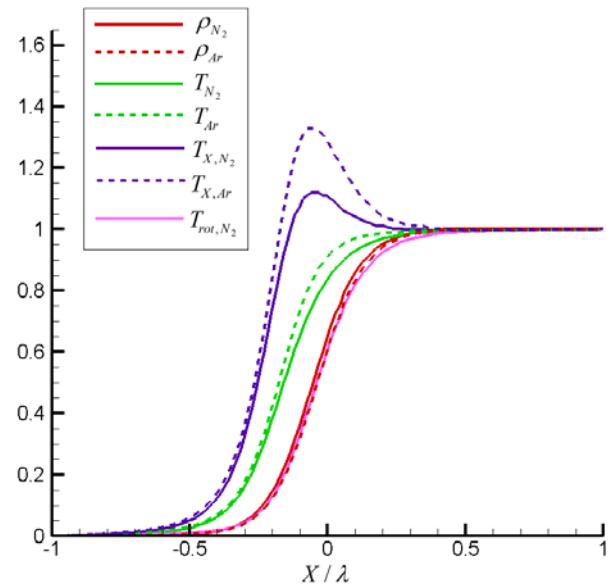


FIG. 10(a) SHOCK WAVE PROPERTIES IN A MIXTURE OF NITROGEN AND ARGON IN TRANSLATIONAL AND ROTATIONAL NON-EQUILIBRIUM WITH 1:1 CONCENTRATION RATIO AT M = 2

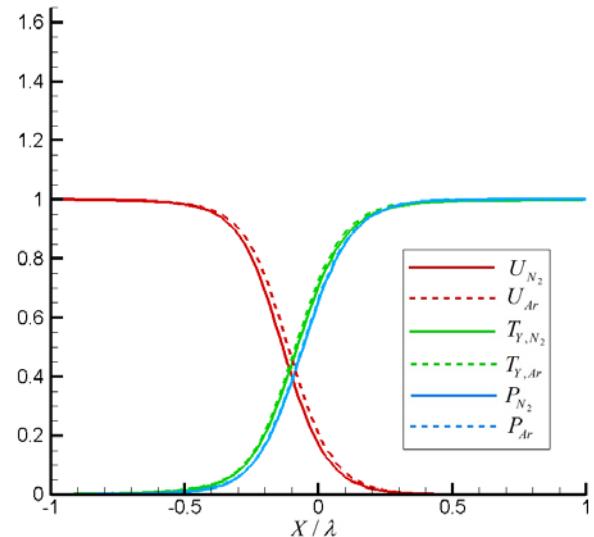


FIG. 10(b) SHOCK WAVE PROPERTIES IN A MIXTURE OF NITROGEN AND ARGON IN TRANSLATIONAL AND ROTATIONAL NON-EQUILIBRIUM WITH 1:1 CONCENTRATION RATIO AT M = 2

Figure 11 and 12 show various flow properties for the two gases at Mach 5 with concentration as in air and for a concentration ratio of 1:1 respectively. These figures are similar to Figs. 9 and 10 in terms of variation of flow properties of the two gases across the shock. However due to higher Mach number, the peaks of normalized longitudinal temperatures and translational temperature of the two gases are much higher and there is greater transfer of rotational energy of nitrogen into translational energy of Argon.

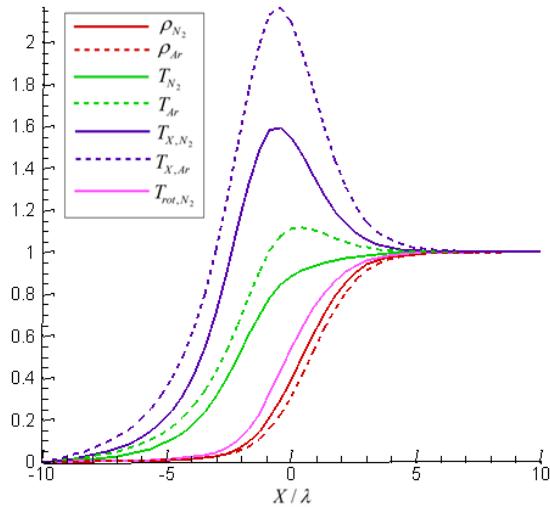


FIG. 11(a) SHOCK WAVE PROPERTIES IN A MIXTURE OF NITROGEN AND ARGON IN TRANSLATIONAL AND ROTATIONAL NON-EQUILIBRIUM WITH AIR CONCENTRATION AT M = 5

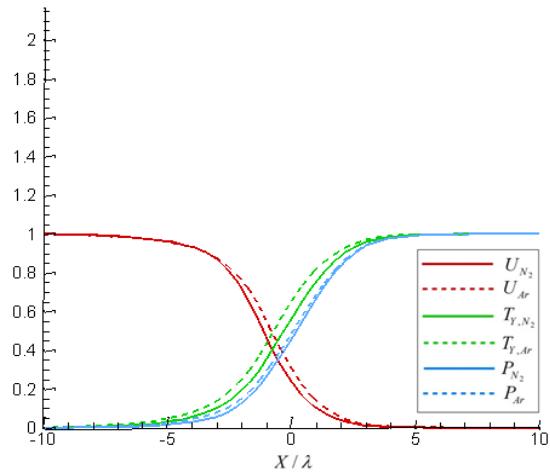


FIG. 11(b) SHOCK WAVE PROPERTIES IN A MIXTURE OF NITROGEN AND ARGON IN TRANSLATIONAL AND ROTATIONAL NON-EQUILIBRIUM WITH AIR CONCENTRATION AT M = 5

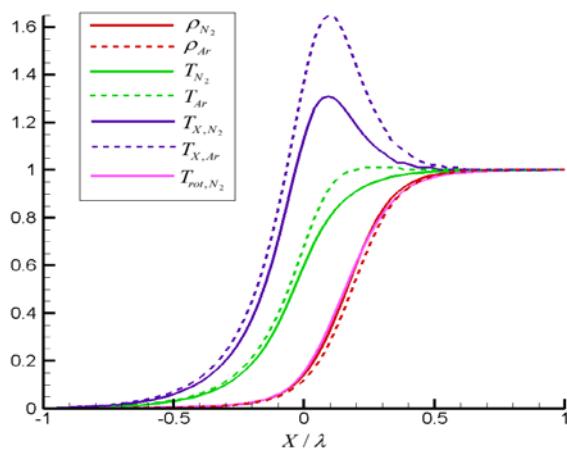


FIG. 12(a) SHOCK WAVE PROPERTIES IN A MIXTURE OF NITROGEN AND ARGON IN TRANSLATIONAL AND ROTATIONAL NON-EQUILIBRIUM WITH 1:1 CONCENTRATION RATIO AT M = 5

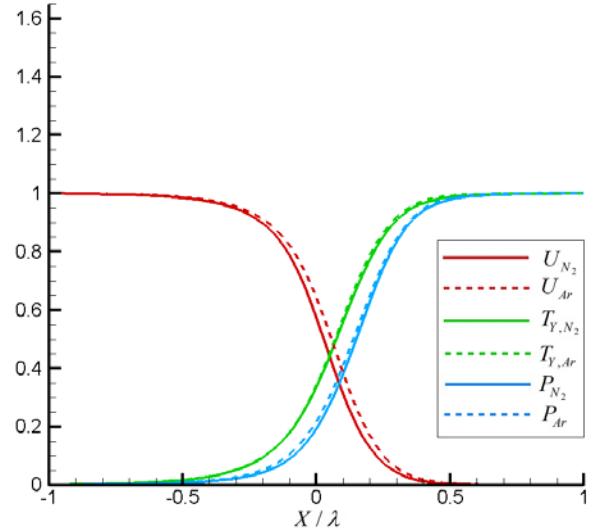


FIG. 12(b) SHOCK WAVE PROPERTIES IN A MIXTURE OF NITROGEN AND ARGON IN TRANSLATIONAL AND ROTATIONAL NON-EQUILIBRIUM WITH 1:1 CONCENTRATION RATIO AT M = 5

## 2) $N_2$ and $O_2$ Mixture

This case is the same as that shown in Fig. 6 except that both  $N_2$  and  $O_2$  are in both translational and rotational non-equilibrium. The mass ratio equals 1.1423 and the diameter ratio equals 0.9156. The gases are again assumed to be non-reacting. Figure 13 shows various flow properties for the two gases across the shock at Mach 2 for air concentration ratio. Again as before in Fig. 6,  $N_2$  being lighter than  $O_2$ , it experiences changes in the shock properties earlier than  $O_2$ . However it is important to note that the peak of the longitudinal component of the translational temperature for  $O_2$  is only slightly higher than that for  $N_2$  in this case compared to that in Fig. 9 where peaks of normalized longitudinal temperature and translational temperature for Ar had much higher value than that for  $N_2$ . It is due to the fact that the mass and diameter ratio of  $N_2$  and  $O_2$  are nearly the same; therefore there is little transfer of energy between the two in the mixture. Figure 14 shows various flow properties for the two gases across the shock at Mach 2 for 1:1 concentration ratio. Compared to Fig. 13, the peaks for the longitudinal component of translational temperature are higher in this case as expected. Figure 15 and 16 show various flow properties for the two gases across the shock at Mach 5 for air concentration ratio and 1:1 concentration ratio respectively. Again the results are similar to those shown in Figs. 13 and 14 except that the peaks for longitudinal component of translation temperature as well as translation

temperature are much higher because of greater Mach number.

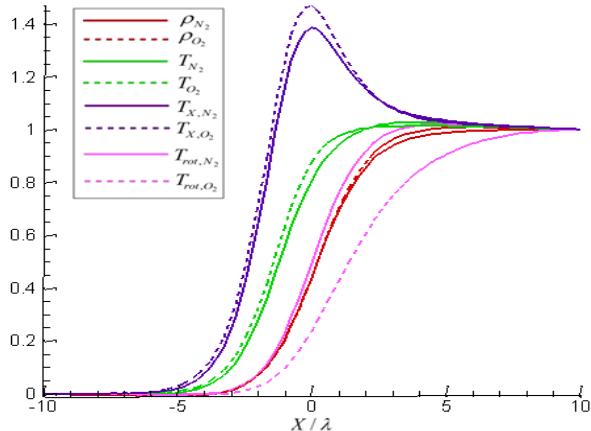


FIG. 13(a) SHOCK WAVE PROPERTIES IN A MIXTURE OF NITROGEN AND OXYGEN IN TRANSLATIONAL AND ROTATIONAL NON-EQUILIBRIUM WITH AIR CONCENTRATION AT M = 2

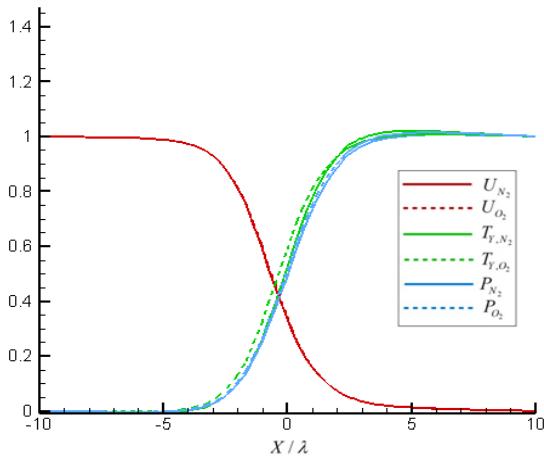


FIG. 13(b) SHOCK WAVE PROPERTIES IN A MIXTURE OF NITROGEN AND OXYGEN IN TRANSLATIONAL AND ROTATIONAL NON-EQUILIBRIUM WITH AIR CONCENTRATION AT M = 2

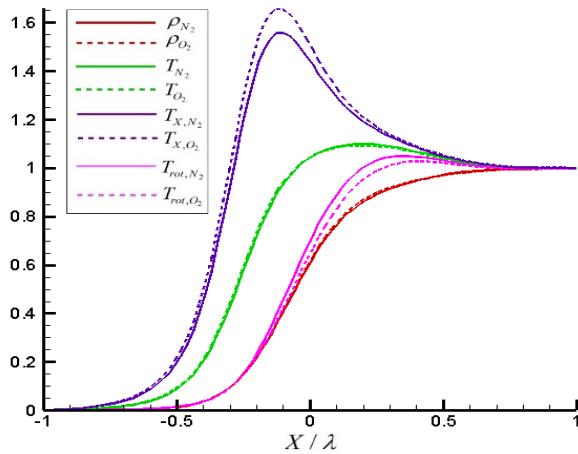


FIG. 14(a) SHOCK WAVE PROPERTIES IN A MIXTURE OF NITROGEN AND OXYGEN IN TRANSLATIONAL AND ROTATIONAL NON-EQUILIBRIUM WITH 1:1 CONCENTRATION RATIO AT M = 2

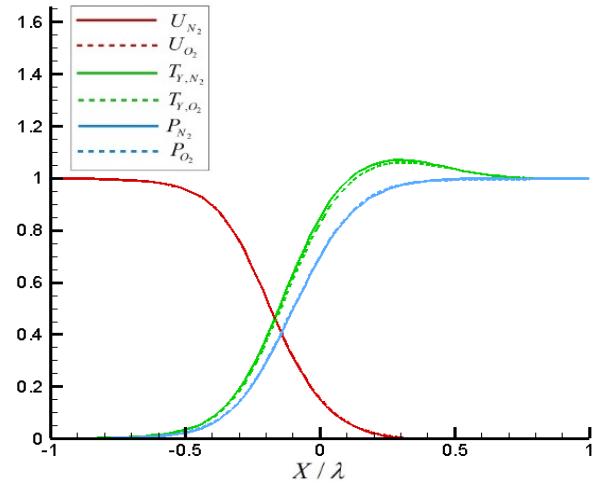


FIG. 14(b) SHOCK WAVE PROPERTIES IN A MIXTURE OF NITROGEN AND OXYGEN IN TRANSLATIONAL AND ROTATIONAL NON-EQUILIBRIUM WITH 1:1 CONCENTRATION RATIO AT M = 2

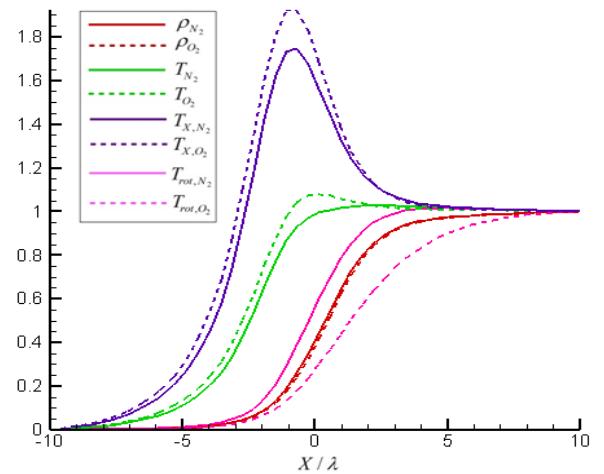


FIG. 15(a) SHOCK WAVE PROPERTIES IN A MIXTURE OF NITROGEN AND OXYGEN IN TRANSLATIONAL AND ROTATIONAL NON-EQUILIBRIUM WITH AIR CONCENTRATION AT M = 5

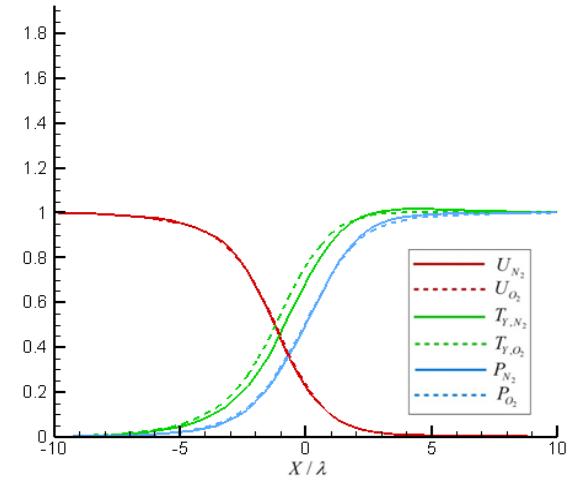


FIG. 15(b) SHOCK WAVE PROPERTIES IN A MIXTURE OF NITROGEN AND OXYGEN IN TRANSLATIONAL AND ROTATIONAL NON-EQUILIBRIUM WITH AIR CONCENTRATION AT M = 5

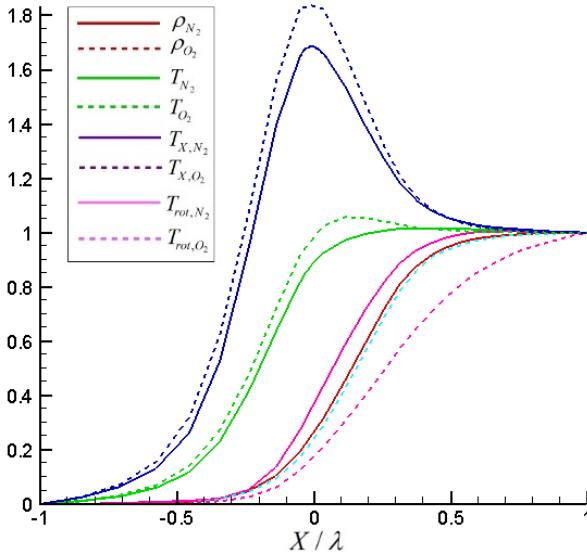


FIG. 16(a) SHOCK WAVE PROPERTIES IN A MIXTURE OF NITROGEN AND OXYGEN IN TRANSLATIONAL AND ROTATIONAL NON-EQUILIBRIUM WITH 1:1 CONCENTRATION RATIO AT M = 5

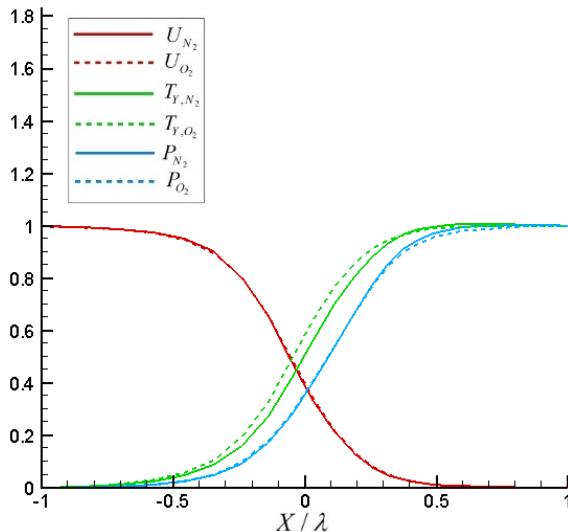


FIG. 16(b) SHOCK WAVE PROPERTIES IN A MIXTURE OF NITROGEN AND OXYGEN IN TRANSLATIONAL AND ROTATIONAL NON-EQUILIBRIUM WITH 1:1 CONCENTRATION RATIO AT M = 5

### *Shock Wave Solutions for Binary Gas Mixture $N_2$ and $O_2$ in Translational, Rotational and Vibrational Non-equilibrium*

#### 1) $N_2$ and $O_2$ Mixture

This case is the same as that shown in Figs. 15 and 16 except that both  $N_2$  and  $O_2$  are now in translational, rotational and vibrational non-equilibrium. The mass ratio equals 1.1423 and the diameter ratio equals 0.9156. The gases are again assumed to be non-reacting. Figure 17 shows various flow properties for the two gases at Mach 5

for air concentration ratio. Again as before in Fig. 15,  $N_2$  being lighter than  $O_2$ , it experiences changes in the shock properties earlier than  $O_2$ . However it is important to note that not only the peak of the longitudinal component of the translational temperature for  $O_2$  is now slightly higher than that for  $N_2$  in this case compared to that in Figure 15 but the magnitude of the peaks of longitudinal component of translational temperature for both  $N_2$  and  $O_2$  is higher than those in Fig. 15. It is due to the transfer of vibrational as well as rotational energy into the translational energy of the two gases. Figure 18 shows various flow properties for the two gases at Mach 5 for air 1:1 concentration ratio.

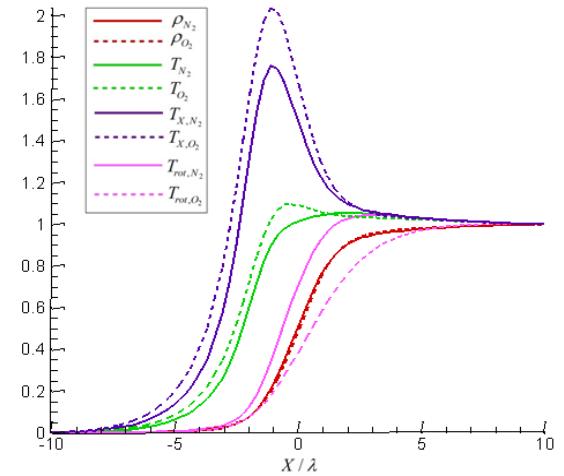


FIG. 17(a) SHOCK WAVE PROPERTIES IN A MIXTURE OF NITROGEN AND OXYGEN IN TRANSLATIONAL, ROTATIONAL AND VIBRATIONAL NON-EQUILIBRIUM WITH AIR CONCENTRATION AT M = 5

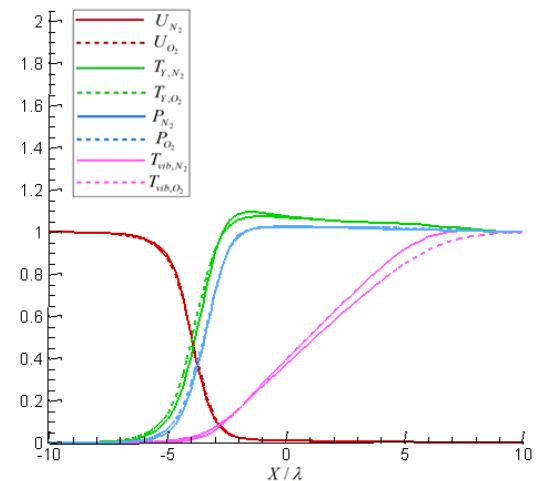


FIG. 17(b) SHOCK WAVE PROPERTIES IN A MIXTURE OF NITROGEN AND OXYGEN IN TRANSLATIONAL, ROTATIONAL AND VIBRATIONAL NON-EQUILIBRIUM WITH AIR CONCENTRATION AT M = 5

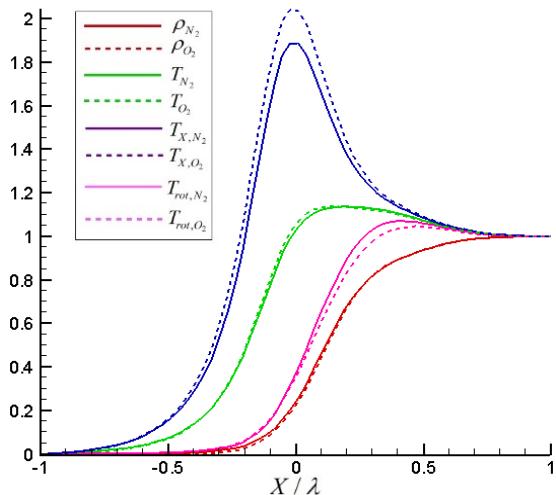


FIG. 18(a) SHOCK WAVE PROPERTIES IN A MIXTURE OF NITROGEN AND OXYGEN IN TRANSLATIONAL, ROTATIONAL AND VIBRATIONAL NON-EQUILIBRIUM WITH 1:1 CONCENTRATION RATIO AT  $M = 5$

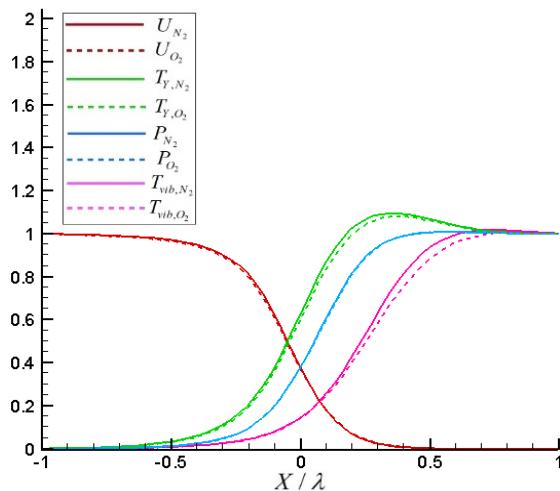


FIG. 18(b) SHOCK WAVE PROPERTIES IN A MIXTURE OF NITROGEN AND OXYGEN IN TRANSLATIONAL, ROTATIONAL AND VIBRATIONAL NON-EQUILIBRIUM WITH 1:1 CONCENTRATION RATIO AT  $M = 5$

## Conclusions

The direct method of Tcheremissine has been applied for solving the Generalized Boltzmann Equation in an impulse space for computation of shock waves in a binary mixture of non-reacting monoatomic and diatomic gases in translational, rotational and vibrational non-equilibrium. The method has been validated by comparing the present solutions with those of Kosuge, Aoki and Takata for a binary mixture of inert monoatomic gases using a different numerical method due to Sone. A parametric study of the performance of the current method has been performed to evaluate its capability for computing shock waves in binary inert mixtures of gases for various mass ratios, concentration ratios, and diameter

ratios. It is demonstrated that the current method is able to handle a wide range of mass, diameter, and concentration ratios without any numerical difficulty. The method is also applied to a non-reacting mixture of two of the air constituents (diatomic Nitrogen, diatomic Oxygen, and monoatomic Argon). The behavior of shock waves in a mixture representative of air constituents is computed. In particular, the computations for a mixture of Nitrogen and Argon in translational and rotational non-equilibrium and for a mixture of Nitrogen and Oxygen in translational, rotational and vibrational non-equilibrium give some interesting insight into the energy transfer process in the mixture. In case of mixture of Argon and Nitrogen, the rotational energy from Nitrogen is transferred into the translational energy of Argon. In case of mixture of Nitrogen and Oxygen, the rotational and vibrational energy of Nitrogen and Oxygen is primarily transferred into their translational energy.

## REFERENCES

- Agarwal, R. K., and TCheremissine, F. G., "Computation of Hypersonic Shock Structure in Diatomic Gases with Rotational and Vibrational Relaxation using the Generalized Boltzmann Equation," AIAA Paper 2008-1269, 46<sup>th</sup> AIAA Aerospace Sciences Meeting, Reno, NV, 7-10 January 2008.
- Beylich, A.E., "Kinetics of Thermalization in Shock Waves," Phys. of Fluids, 14 (2002): 2683- 2699.
- Chen, R., Agarwal, R. K., and Tcheremissine, F. G., "Computation of Hypersonic Flow of a Diatomic Gas in Rotational Nonequilibrium Past a Blunt Body Using the generalized Boltzmann Equation," AIAA Paper 2007-4550, 39<sup>th</sup> AIAA Thermophysics Conference, Miami, FL, 25-28 June 2007.
- Chen, R., Agarwal, R. K., and Tcheremissine, F. G., "Computation of Supersonic Flow Past 2D Blunt Bodies Using a Boltzmann Solver," AIAA Paper 2005-1102, 43<sup>rd</sup> AIAA Aerospace Sciences Meeting, Reno, NV, Jan. 10-13, 2005.
- Kosuge, S., Aoki, K., and Takata, S., "Shock-Wave Structure for a Binary Gas Mixture: Finite-Difference Analysis of the Boltzmann Equation for Hard-Sphere Molecules," European Journal of Mechanics B – Fluids, 20 (2001): 87-126.
- Raines, A., "A Method for Solving Boltzmann Equation for a

- Gas Mixture in the Case of Cylindrical Symmetry in the Velocity Space," *Comp. Math. and Math. Phys.*, 42 (2002): 1212-1223.
- Sone, Y., *Kinetic Theory and Fluid Dynamics*, Boston: Birkhäuser, 2002.
- Tcheremissine, F. G., Agarwal, R. K., and Wilson, C. D., "A Two-Level Kinetic Model for Rotational- Translational Relaxations in a Diatomic Gas," AIAA Paper 2008-3932, 38<sup>th</sup> AIAA Fluid Dynamics Conference, Seattle, Washington, 23-26 June 2008.
- Tcheremissine, F. G., "Conservative Evaluation of Boltzmann Collision Integral in Discrete Ordinates Approximation," *Computers and Mathematics with Applications*, 35 (1998): 215-221.
- Tcheremissine, F.G., "Solution of the Wang-Chang-Uhlenbeck Master Equation," *Doklady Physics*, 47 (2002): 872-875.
- Wilson, C. D., Agarwal, R. K., and Tcheremissine, F.G., "Computation of Hypersonic Shock Waves in Inert Gas Mixtures Using the Generalized Boltzmann Equation," AIAA Paper 2011-3134, AIAA 42<sup>nd</sup> Thermophysics Conference, Hawaii, 27-30 June 2011.